# Rhodium virtually screens drugs for coronavirus research

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Drug discovery software at Southwest Research Institute is expanding the capacity to virtually screen drug compounds for possible treatment of coronavirus and other infectious diseases.

SwRI's Rhodium virtual screening tool recently evaluated 2 million drug compounds in a few days, hoping to identify high-probability drugs that may have efficacy against the coronavirus with minimal adverse side effects. Institute scientists initiated the molecular modeling research with SwRI internal funding.

"In line with SwRI's mission of developing medical countermeasures for both natural and manmade threats, we are using this proprietary molecular modeling software to help the research community screen drug candidates for future coronavirus research," said Dr. Jonathan Bohmann, an SwRI principal scientist leading the research.

Based on the modeling results, SwRI will team with local research partners, including the Texas Biomedical Research Institute, for the next phase of studies to determine the most efficacious candidates for further drug development and ultimate deployment to virus-affected regions.

Prior to the recent coronavirus outbreak, SwRI increased the capacity of its Rhodium software to scan 250,000 drug compounds per day, up from its prior limit of 25,000. Researchers enhanced the capability with new graphical processing, software updates and machine learning techniques. A 3-D model of a coronavirus was used to evaluate potential drugs from a vast library of compounds.

"This advanced processing capability is demonstrating that virtual screening can rapidly increase the pace of drug discovery, especially in pandemic situations," said Dr. Shawn Blumberg, an SwRI research scientist assisting with the effort.

Virtual screening applies computational techniques to evaluate small molecules and predict how protein structures in infectious diseases will bind with drug compounds. Drug makers have been turning to computational screening as a safe, efficient and cost-effective alternative to evaluating physical samples in a laboratory in the early stages of drug development.

"Rhodium, for example, can be used to find highly probable compounds from databases with hundreds of thousands of drug candidates prior to bench testing in a laboratory," Bohmann added.

Rhodium uses drug compound libraries to predict how protein structures in infectious diseases will bind with compounds or a series of compounds known as ligands. Rhodium's high throughput 3-D analysis of protein docking efficiently selects ligands to predict how a compound interacts with the protein structure. Its machine learning tools interpret rank order analysis of results for faster data analysis.

SwRI scientists use Rhodium to interpret binding data from X-ray crystallography, a technique

commonly used to obtain the 3-D structure,
visualizing how it bonds with a protein.

Provided by Southwest Research Institute

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